

524


Scientific and Technical Information Center

4E12

Title of Invention: FELBAMATE DERIVED COMPOUNDS

Inventors (please provide full names): TIMOTHY L. Macdonald

Earliest Priority Filing Date: 2/9/1994



$$R_2 \equiv \text{Halogen}$$

$$R_3 = \text{OH}$$

$$\text{or } -\text{O-C(=O)-CH}_3$$

Need info @ cpls, components & use for
Treating NEUROLOGICAL DISORDER, TISSUE Damage
Need: d flub hit its abt told in CAPLUS
Copy of claims attached TIT
JES
1624

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Vendors and cost where applicable

Searcher: Sicynane NA Sequence (#) _____ STN _____
 Searcher Phone #: 308-4499 AA Sequence (#) _____ Dialog _____
 Searcher Location: _____ Structure (#) _____ Questel/Orbit _____
 Date Searcher Picked Up: _____ Bibliographic _____ Dr. Link _____
 Date Completed: 10/18/02 Litigation _____ Lexis/Nexis _____
 Searcher Prep & Review Time: _____ Fulltext _____ Sequence Systems _____
 Clerical Prep Time: _____ Patent Family _____ WWW/Internet _____
 Online Time: _____ Other _____ Other (specify) _____

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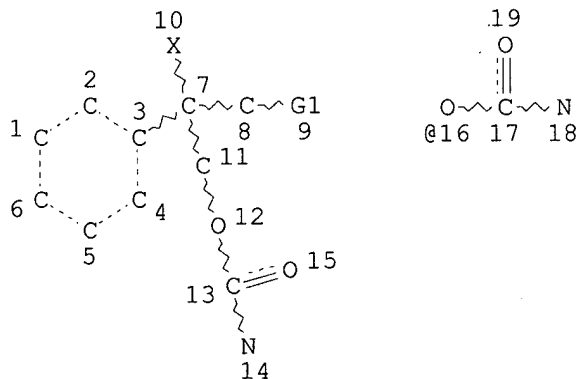
FILE COVERS 1907 - 18 Oct 2002 VOL 137 ISS 17
 FILE LAST UPDATED: 17 Oct 2002 (20021017/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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 L1 STR



VAR G1=OH/16
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
 L3 4 SEA FILE=REGISTRY SSS FUL L1
 L4 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

=> d ibib abs hitstr 14 1-3

L4 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:833070 HCAPLUS

DOCUMENT NUMBER: 135:352836

TITLE: Felbamate-derived compounds for the treatment of neuropathic pain and other conditions

INVENTOR(S): MacDonald, Timothy L.

PATENT ASSIGNEE(S): University of Virginia Patent Foundation, USA

SOURCE: PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001085149	A2	20011115	WO 2001-US14594	20010504
WO 2001085149	A3	20020530		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-202145P P 20000505

OTHER SOURCE(S): MARPAT 135:352836

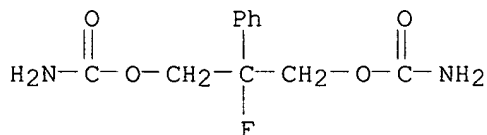
AB The invention discloses the use of felbamate derivs. to treat neuropathic pain, obesity, glaucoma, depression, and mood disorders, as well as other conditions. Prepn. and testing of fluoro derivs. of felbamate are included.

IT **726-99-8P 288302-42-1P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(felbamate-derived compds. for treatment of neuropathic pain and other conditions)

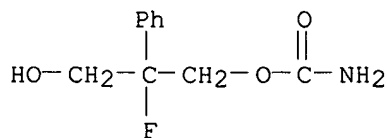
RN 726-99-8 HCAPLUS

CN 1,3-Propanediol, 2-fluoro-2-phenyl-, dicarbamate (9CI) (CA INDEX NAME)



RN 288302-42-1 HCAPLUS

CN 1,3-Propanediol, 2-fluoro-2-phenyl-, monocarbamate (9CI) (CA INDEX NAME)



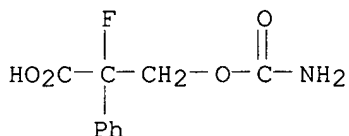
IT 288302-43-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction; felbamate-derived compds. for treatment of neuropathic pain and other conditions)

RN 288302-43-2 HCAPLUS

CN Benzeneacetic acid, .alpha.-[[(aminocarbonyl)oxy]methyl]-.alpha.-fluoro-(9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:573661 HCAPLUS

DOCUMENT NUMBER: 133:172201

TITLE: Felbamate derived compounds

INVENTOR(S): MacDonald, Timothy L.; Miller, Thomas A.; Thompson, Charles D.

PATENT ASSIGNEE(S): University of Virginia Patent Foundation, USA

SOURCE: PCT Int. Appl., 44 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000047202	A1	20000817	WO 2000-US3147	20000208
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1156798	A1	20011128	EP 2000-907199	20000208
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRIORITY APPLN. INFO.: US 1999-119254P P 19990209
 US 1999-136881P ✓ P 19990601
 US 1999-137204P ✓ P 19990602
 WO 2000-US3147 W 20000208

OTHER SOURCE(S): MARPAT 133:172201

AB The present invention relates to novel felbamate derivs. and their use to treat neurol. diseases such as epilepsy and to treat tissue damage resulting from ischemic events. The felbamate derivs. are modified to prevent the formation of metabolites that are believed responsible for the toxicity assocd. with felbamate therapy.

IT 288302-42-1P

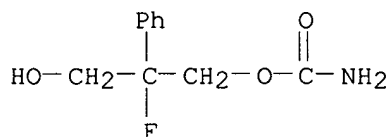
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(felbamate derived compds. to treat neurol. diseases such as epilepsy)

and tissue damage resulting from ischemic events in relation to detn.
of felbamate and its metabolites in urine and toxicity)

RN 288302-42-1 HCAPLUS

CN 1,3-Propanediol, 2-fluoro-2-phenyl-, monocarbamate (9CI) (CA INDEX NAME)



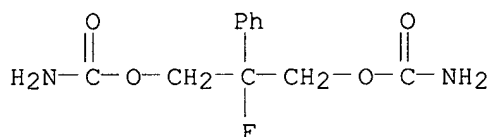
IT 726-99-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(felbamate derived compds. to treat neurol. diseases such as epilepsy and tissue damage resulting from ischemic events in relation to detn. of felbamate and its metabolites in urine and toxicity)

RN 726-99-8 HCAPLUS

CN 1,3-Propanediol, 2-fluoro-2-phenyl-, dicarbamate (9CI) (CA INDEX NAME)



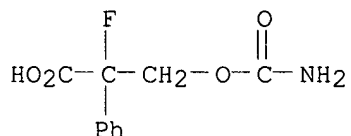
IT 288302-43-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(felbamate derived compds. to treat neurol. diseases such as epilepsy and tissue damage resulting from ischemic events in relation to detn. of felbamate and its metabolites in urine and toxicity)

RN 288302-43-2 HCAPLUS

CN Benzeneacetic acid, .alpha.-[[(aminocarbonyl)oxy]methyl]-.alpha.-fluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1987:597737 HCAPLUS

DOCUMENT NUMBER: 107:197737

TITLE: Metabolites of felbamate: synthesis of
2-(4-hydroxyphenyl)-1,3-propanediol dicarbamate,
2-phenyl-2-hydroxy-1,3-propanediol dicarbamate, and
2-phenyl-1,3-propanediol monocarbamate

AUTHOR(S): Choi, Yong M.; Kucharczyk, Norbert; Sofia, R. Duane

CORPORATE SOURCE: Wallace Lab. Div., Carter-Wallace. Inc., Cranbury, NJ,
08512, USA

SOURCE: Tetrahedron (1986), 42(23), 6399-404

CODEN: TETRAB; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 107:197737

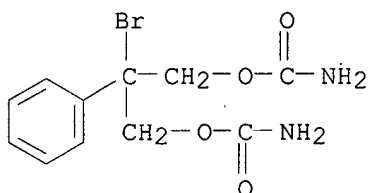
AB Three major metabolites of felbamate, 4-HOC6H4CH(CH2O2CNH2)2 (I), HOCPh(CH2O2CNH2)2 (II), and HOCH2CHPhCH2O2CNH2 (III) were prepd. Carboxylation of 4-RC6H4CR1R2R3 (IV, R = OMe, R1 = R2 = H, R3 = CO2H) followed by redn. gave IV (R = OMe, R1 = H, R2 = R3 = CH2OH), which was phosgenated, demethylated, and carbamoylated to give I. Phosgenation of IV (R = R1 = H, R2 = R3 = CH2OH) followed by bromination and carbamoylation gave IV (R = H, R1 = Br, R2 = R3 = CH2O2CNH2), which was cyclized and aminolyzed to give II. III was prepd. by methylation of IV (R = R1 = H, R2 = R3 = CH2OH), followed by phosgenation, carbamoylation, and demethylation.

IT 109482-30-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and ring closure of)

RN 109482-30-6 HCAPLUS

CN 1,3-Propanediol, 2-bromo-2-phenyl-, dicarbamate (9CI) (CA INDEX NAME)



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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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=> s 13

L5 1 L3

=> d all 15 1

L5 ANSWER 1 OF 1 CAOLD COPYRIGHT 2002 ACS

AN CA58:6756f CAOLD

TI light-sensitive purpurogallin derivs.

AU Uhlig, Fritz; Endermann, F.; Neugebauer, W.
 DT Patent
 TI purpurogallin derivs. (light-sensitive)
 PA Azoplate Corp.

DT Patent
 PATENT NO. KIND DATE

PI US 3061430 1962
 IT 682-33-7 682-72-4 726-99-8 1510-41-4 2708-70-5
 23311-62-8 100065-32-5 103936-55-6 103936-56-7 106279-63-4

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 DICTIONARY FILE UPDATES: 16 OCT 2002 HIGHEST RN 462058-01-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

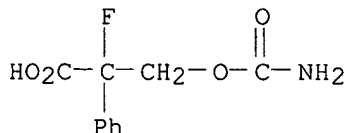
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 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
 PROPERTIES for more information. See STNote 27, Searching Properties
 in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d ide can 13 1-4

L3 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2002 ACS
 RN 288302-43-2 REGISTRY
 CN Benzeneacetic acid, .alpha.-[[(aminocarbonyl)oxy]methyl]-.alpha.-fluoro-
 (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C10 H10 F N O4
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER



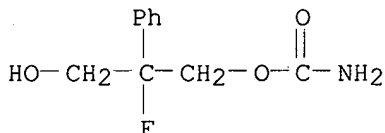
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 135:352836

REFERENCE 2: 133:172201

L3 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2002 ACS
 RN 288302-42-1 REGISTRY
 CN 1,3-Propanediol, 2-fluoro-2-phenyl-, monocarbamate (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C10 H12 F N O3
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER



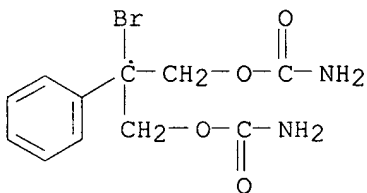
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 135:352836

REFERENCE 2: 133:172201

L3 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2002 ACS
 RN 109482-30-6 REGISTRY
 CN 1,3-Propanediol, 2-bromo-2-phenyl-, dicarbamate (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C11 H13 Br N2 O4
 SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
 (*File contains numerically searchable property data)



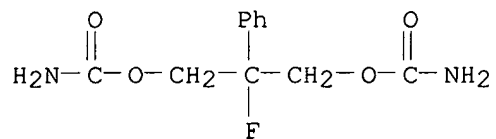
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 107:197737

L3 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2002 ACS
 RN 726-99-8 REGISTRY
 CN 1,3-Propanediol, 2-fluoro-2-phenyl-, dicarbamate (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Carbamic acid, 2-fluoro-2-phenyltrimethylene ester (7CI, 8CI)

FS 3D CONCORD
MF C11 H13 F N2 O4
LC STN Files: CA, CAOLD, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 135:352836

REFERENCE 2: 133:172201